

Energy dependence of mass distributions in fragmentation

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We study fragmentation numerically using a simple model in which an object is taken to be a set of particles that interact pairwise via a Lennard-Jones potential while the effect of the fragmentation-induced forces is represented by some initial velocities assigned to the particles. The motion of the particles, which is given by Newton's laws, is followed by molecular dynamics calculations. As time evolves, the particles form clusters which are identified as fragments. The steady-state cumulative distribution of the fragment masses is studied and found to have an effective power-law region. The power-law exponent increases with the energy given to the particles by the fragmentation-induced forces. This result is confirmed by experiments.

keywords: Fragmentation; Mass distributions; Energy dependence

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I. INTRODUCTION

Fragmentation is a common physical process that occurs in everyday life and in many areas of science and technology. When an object experiences an impact or a shock in which it receives sufficient energy, it will break up into many smaller pieces or fragments. Although fragmentation is a complex process that involves propagation of many cracks and their interaction, some simple overall statistical features have been observed. A large amount of data have been collected which indicate that for a wide variety of fragmented objects, ranging from sand and gravels to asteroids, the cumulative distribution of sizes can be represented by a power law for some non-negligible range [1]. Such feature was also found in the cumulative distribution of fragment volumes in the brittle fracture of glass spheres [2].

Fragmentation of long glass rods dropped onto the floor [3] showed that the distribution of fragment masses changes from lognormal to one with a power-law region when the dropping height is large enough. Oddershede, Dimon and Bohr [4] studied fragmentation of objects made of different materials including gypsum, soap, and potato, and reported that the cumulative fragment mass distribution can be fitted by a power law with an exponential cutoff. Moreover, the cumulative distribution was found to be insensitive to the types of the material with the power-law exponent depending only on the morphology of the objects. These observations were interpreted [4] as evidence that the fragmentation process is a self-organized critical phenomenon and that the power-law exponent depends only on the effective dimension of the objects. In a later study using plates of dry clay, Meibom and Balslev [5] observed instead that the cumulative fragment mass distribution has two power-law regions and a cutoff, with the exponent larger for the smaller fragments. Moreover, the two regions were found to be separated by a mass whose value increases with the thickness of the clay plates. Based on these results, they concluded [5] that the power-law exponent depends on the dimensionality of the original object on the scale of the fragment considered and not simply on the global dimensionality of the object. Both experimental studies [4,5] indicate that the power-law exponent increases with dimensionality.

Geometric statistical models [6,7] for fragmentation have been studied in which the fragments are produced according to an assumed distribution of pre-existing fracture points, lines or planes in one, two or three dimensions. The fragment size distribution depends on the form of the distribution of the pre-existing flaws. For example, the cumulative fragment size distribution will be exponential [7] for an one-dimensional object if the fracture points obey a Poisson distribution. Another approach is to describe the fragmentation process by a rate equation [8]. Power-law fragment mass distributions can be obtained when the relative breakup rate is taken to be a power-law form. A third approach considers fragmentation of an object as a partition of a set of particles. This is mathematically equivalent to the partition of an integer [9]. When each partition is assumed to be equally likely, the actual distribution would be the one that can be realized in the largest number of ways which can be obtained by maximizing the information entropy [10,11]. On the other hand, different weights could be assigned to the partitions to get different fragment size distributions [12].

Various models have been introduced to study fragmentation numerically [13–16]. Inaoka and Takayasu [13] modeled the impact fracture process as a competitive growth of fragments. Together with Toyosawa, they found that the fragment mass distribution depends on how the object is hit when the object has an aspect ratio other than one. The distribution shows a power law with a flat region then a cutoff when the object is hit by its thin side but a power law with a cutoff when it is hit by its broad side [17]. The former results resemble the experimental observation of two power-law regions [5] discussed earlier. In the other models, an object is described by an assembly of basic constituents or building blocks which are connected to each other via elastic springs or beams [14,15], or by some history-dependent attractive force [16]. The object is then subjected to some external force [14,15] or the constituents be given some initial random velocities from a uniform distribution with a maximum value [16] and the whole system evolves according to Newtonian dynamics. The connection or bond between the constituents is taken to be broken when some specific rules are satisfied. Fragment mass distributions with a power-law region were found in these numerical studies (except when the object is broken under both compression and elongation [15]) and this result is robust to variation in the parameters of the models.

In this paper, we study how the fragment mass distribution depends on the input energy imparted by forces that cause the fragmentation. Such a dependence was suggested in Ref. [16] in which the power-law exponent was found to change considerably when the maximum velocity in the uniform distribution is around 1. However, as discussed in that reference, it was not clear that whether the dependence is continuous as the maximum velocity is varied or whether there is a crossover from other values of the maximum velocity to the value of 1. To study such dependence in detail, we use a simple model of fragmentation in which we can vary the input energy easily. The model used is described in Sec. II. Results obtained are presented in Sec. III and we shall see that there is a continuous change in the power-law exponent as the input energy is increased. In Sec. IV, we discuss our results and compare them to some experimental observations. The paper ends with a conclusion in Sec. V.

II. THE MODEL

A model of fragmentation should contain at least two aspects: a description of the object to be fractured and a representation of the effect of the fracturing forces. The simplest model of an object is that it consists of N particles. In order for the object to remain as a whole piece but without collapsing to a point, the particles should attract one another when they are far away but repel each other when they are too close. A convenient choice of such an interaction is the Lennard-Jones potential:

$$V(r) = \frac{K_1}{r^{12}} - \frac{K_2}{r^6}, \quad (1)$$

with r being the separation between the particles. To speed up the calculations, the interaction potential V is truncated when r is three times the equilibrium separation σ . The parameters K_1 and K_2 are fixed to be 5 and 10 respectively, and σ is thus 1 unit. We have checked that the truncation does not affect the results for the fragment mass distributions. Every particle is taken to have the same mass of 1 unit. In order to obtain a statistically significant number of fragments and at the same time without making N formidably large computationally, we study two-dimensional objects. The initial positions of the particles are chosen at random inside a square whose size is set by the number density ρ . A snapshot of the initial configuration of the particles is shown in Fig. 1.

A major effect of the impact or shock that causes fragmentation is to impart energy to the object. With the imparted energy, bonds are broken and, as a result, the object breaks up into pieces. This effect of the fragmentation-induced forces is represented by assigning the particles some initial velocities as was done in Ref. [16]. In this spirit, different situations of fragmentation can be studied by assigning different distributions of initial velocities to the particles.

The fragmentation process is followed using molecular dynamics calculations which were introduced to study fragmentation by Holian and Grady [18]. To compare with experiments, we use a free boundary condition instead of an expanding periodic boundary condition as used in their study. Each particle moves according to Newton's laws of motion. At each time step, the positions and velocities are updated for all the particles at the same time by the Verlet algorithm [19]. Both the total momentum and the total energy, which is the sum of the potential and kinetic energies, of the particles are conserved during the fragmentation process. Momentum conservation is automatic in the Verlet algorithm while energy conservation is enforced in our numerical scheme [20].

III. RESULTS

We first report results for the case when the particles are given some initial radial velocities. The magnitude of the velocity is proportional to the distance of the particle from the center of the square:

$$\begin{aligned} v_{xi} &= Cx_i \\ v_{yi} &= Cy_i \end{aligned} \quad (2)$$

where x_i and y_i are the distances of the i -th particle from the center along the x and y -directions. This velocity distribution was also studied in Ref. [15,18], and might be realized in fragmentation of metal rings that were forced to undergo rapid radial expansion through the application of an impulsive magnetic load [21] or in explosive munitions tests [22]. Besides the radial velocities, each particle has also a small thermal random velocity. The thermal kinetic energy is always less than the kinetic energy of the assigned velocities.

In this model, the input energy imparted by the fracturing forces can be easily measured by the kinetic energy due to the assigned initial velocities. Therefore, we vary the value of the proportionality constant C in (2) to change the input energy. The initial configuration of the particles is kept fixed so that the initial potential energy of the system remains constant. The random thermal energy is also kept fixed. Thus, a convenient parameter to describe the situations of different input energies is the ratio of the initial kinetic energy to the absolute value of the initial potential energy of the particles, which we denote as R . Snapshots of the configuration of the particles for $R = 0.43$ at some later times are shown in Fig. 2. It can be seen that the particles distribute themselves in clusters of various sizes. Particles that are located within a distance $d = 3.0 \sigma$ of one another are naturally defined to be in one fragment. The mass of each fragment is equal to the number of particles in the fragment as we have taken the mass of each particle to be one unit.

To study the statistical features of the fragmentation process, we calculate the cumulative mass distribution. Denote the distribution of fragments of mass m by $n(m)$, the cumulative distribution $F(m)$ is defined as

$$F(m) = \int_m^\infty n(m') dm' \quad (3)$$

which measures the number of fragments whose mass larger than m . We calculate $F(m)$ regularly and find that it becomes steady after a certain large enough number of time steps (about 5000 time steps for a time step of 0.01). The steady-state cumulative distributions $F(m)$ are analyzed. All the results reported below refer to the steady-state distributions.

In Fig. 3, we show $F(m)$ for $R = 0.43$ and $N = 4200$. A short effective power-law region which extends for about a decade can be observed:

$$F(m) \sim m^{-\alpha} \quad (4)$$

for intermediate fragment masses. The power-law exponent α is found to be 0.41 by fitting the best straight line region in the log-log plot. This power-law region is verified by the existence of a plateau in the plot of $F(m)m^\alpha$ versus m as shown in the inset of Fig. 3. We have checked that the results do not change much if d is in the range of 1.5 to 3.0σ . The extent of the power-law region is longer when we use a larger N . It follows from (3) that $n(m)$ also has a power-law region whose exponent is given by $\alpha + 1$, i.e., $n(m) \sim m^{-(\alpha+1)}$.

In Fig. 4, we plot the cumulative mass distributions for various values of R from 0.43 to 6.49. As R increases, $F(m)$ changes. The fragment mass distribution is thus not universal. Specifically, the power-law region shrinks and the exponent α increases as R increases. (For the largest value $R = 6.49$, the power-law region barely exists.) The dependence of α on R is plotted in Fig. 5. As the input energy increases, we find the average fragment mass decreases as expected. In Ref. [18], $F(m)$ is fitted by a sum of two exponentials. We find that this form works for small values of R but not for intermediate values of R . A decrease in the average fragment mass with C was also reported in Ref. [18] but the dependence of $F(m)$ on C was not presented.

We have tested the robustness of our result by changing various parameters in the model [20]. Initial configurations corresponding to different values of the number density ρ have been studied. Different values of N have been used. Furthermore, particles initially confined inside a circular region have also been studied. The same result that the exponent of the power-law region of $F(m)$ increases with R (for values of R not too large; see below) is observed in all these different cases.

Seeing the exponent increases with the input energy, a natural question is whether the power-law behavior will continue in the limit of very large input energy. In our numerical study, we find that when R is larger than a certain value, there is no longer any discernable power-law region in $F(m)$. In the limit of very large R ($R > 100$), $F(m)$ becomes exponential. However, for such large values of R , the average mass of the fragments is only about 2. This suggests that a larger N has to be used for such explorations. Since calculations with a large N are computationally expensive, this question would be more easily addressed by experimental studies [24].

We have also investigated the effect of the form of the initial assigned velocities on the mass distribution by studying the case when only velocities with random direction are assigned to the particles [16]. This case corresponds physically to the object being heated up. When the velocities are small or the temperature is low, the object remains mainly as a whole piece as expected. As the magnitude of the velocities increases, we find that an effective power-law region also develops in $F(m)$ but with a shorter extent as compared to that for radial initial velocities. It would be interesting to study experimentally whether power law could indeed be observed in the distributions of fragments resulting from thermal dissociation.

IV. DISCUSSION

A possible dependence of the power-law exponent on input energy has been hinted by earlier experiments [3,23]. To test this result directly, we have performed experiments of long glass rods dropped onto the floor similar to those reported in Ref. [3] specifically to check the dependence of the fragment distributions on the input energy. Details of the experiment will be reported elsewhere [24]. Here, we shall outline the main experimental observations and compare them with our simulation results.

Potential energy is lost as the glass rod is dropped from a height onto the floor. If all the energy is imparted to the glass rod when it reaches the floor and causes it to break up into fragments, then the input energy will be proportional to the height of the fall. Thus, the glass rods are dropped from various heights and the corresponding distributions of the fragment masses analyzed. The power-law region is again found to shrink as the height increases. Moreover, the exponent α increases from about 0.3 to 0.8 for heights of fall ranging between 1.2 m to 10.6 m similar to that observed in the simulation.

If the power law in the fragment mass distribution is a result of some self-organizing effect of the dynamics of the fragmentation process, one would expect that the exponent should not depend on how much the system is driven or, in other words, how much the input energy is. Thus, a dependence of the exponent on the input energy suggests that

the fragmentation of glass rods on dropping onto the floor is not a self-organized critical phenomenon, contrary to that suggested in Ref. [4].

A dependence of the power-law on input energy was also found in an analytical model of fragmentation recently studied by Marsili and Zhang [25]. In their model, fragmentation is assumed to happen in a hierarchical order and at each level of the hierarchy, a fragment will break further or not into two smaller pieces depending on whether or not its energy density exceeds a certain threshold. They found that the distribution of fragment sizes has an effective power law with the effective exponent increases with the input energy, and equals to the dimension of the object in the limit of very large input energy. There is, however, no obvious hierarchical order in the breaking of the object in our model.

V. CONCLUSION

We have studied a simple model of fragmentation numerically using molecular dynamics calculations. The two essential physical ingredients of the model are: (i) the consideration of an object as a set of particles that interact with each other pairwise via a truncated Lennard-Jones potential and (ii) the approximation of the effect of abruptly applied fracturing forces by some specified initial velocities assigned to the particles. Although the model is simple, the fragment mass distribution obtained displays some features observed in experiments. First, there is an effective power-law region for a range of input energies. The origin of such power laws can be seen as a result of the competition between the forces that tend to break up an object and the cohesive forces that keep the object as a whole when the two kinds of forces do not differ too much in magnitude. Second, the effective exponent increases with the input energy, as observed in the experiments of dropping glass rods onto the floor [24]. This second feature suggests that the impact fragmentation process is not a self-organizing phenomenon. Our study thus sheds light on why power-law behaviour is so overwhelmingly persistent in the observation of fragment distributions and why a range of power-law exponents has been reported.

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FIGURE CAPTIONS

FIG. 1. The initial configuration of the particles for $N = 4200$ and $\rho = 0.61$. The coordinates are measured in arbitrary units; for comparison, the equilibrium separation between two particles is 1 unit.

FIG. 2. The configuration of the particles at (a) 1000 and (b) 5000 time steps for the same parameters in Fig. 1 and $R = 0.43$.

FIG. 3. The cumulative distribution of fragment masses $F(m)$ versus m for the same parameters in Fig. 2. m is measured in terms of the mass of 1 particle which is taken to be 1 unit. An effective power-law region of about a decade is observed and is fitted by the solid line with an exponent α equals to 0.41. In the inset, we plot $F(m)m^\alpha$ versus m , the existence of a plateau region supports the power-law behavior.

FIG. 4. The cumulative distribution of fragment masses $F(m)$ versus m for various values of R . $R = 0.43$ (circles), $R = 1.19$ (squares), $R = 2.45$ (rhombuses), $R = 4.22$ (triangles), and $R = 6.49$ (triangles). The power-law region shrinks and the exponent α increases generally as R increases.

FIG. 5. The R -dependence of the power-law exponent α for the cases shown in Fig. 4.

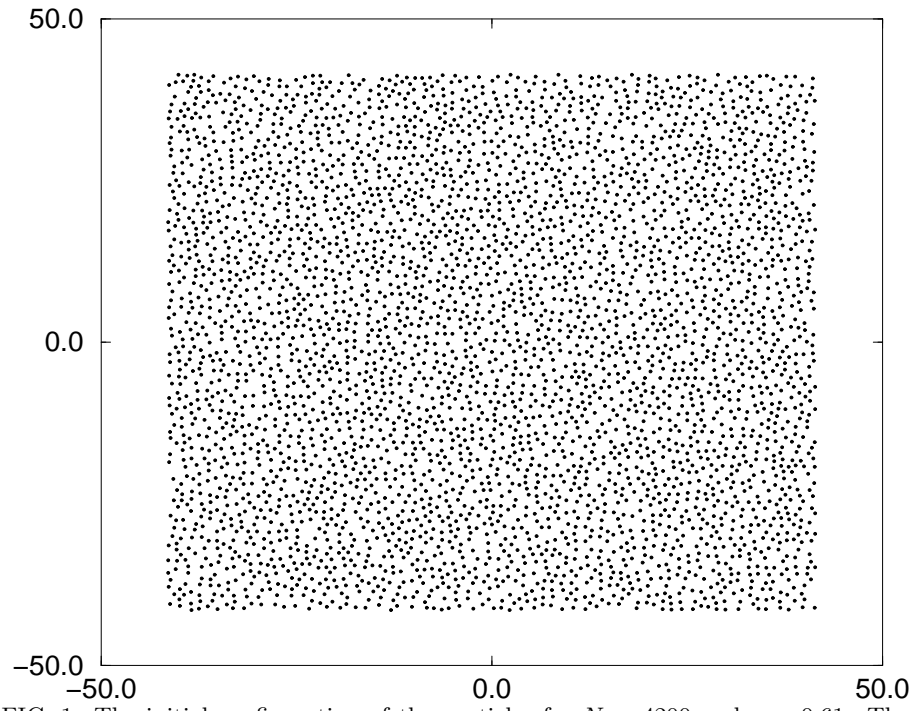


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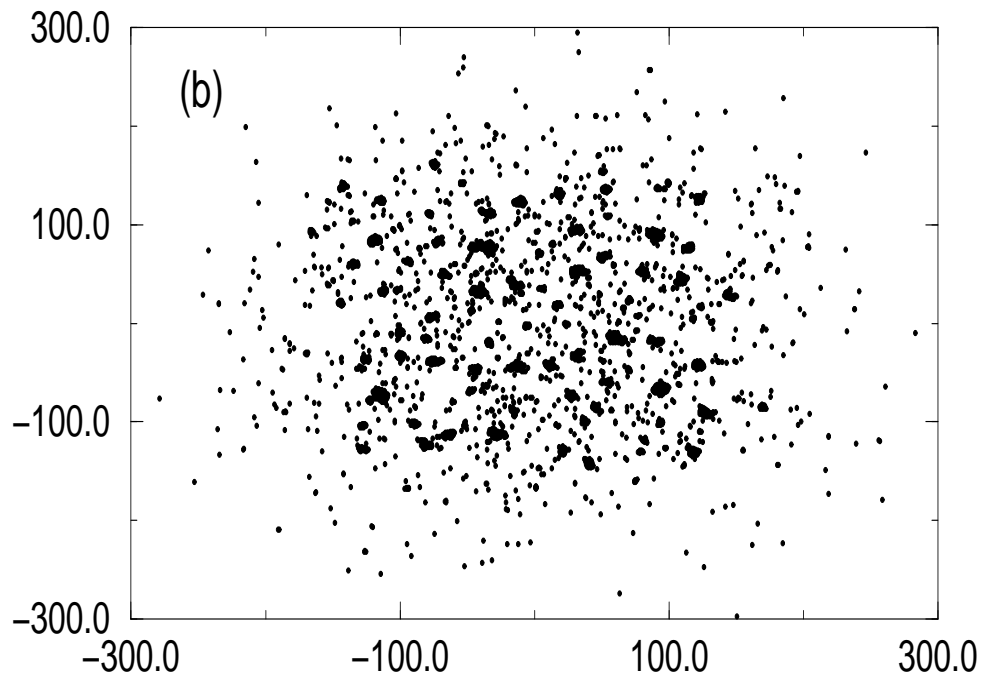
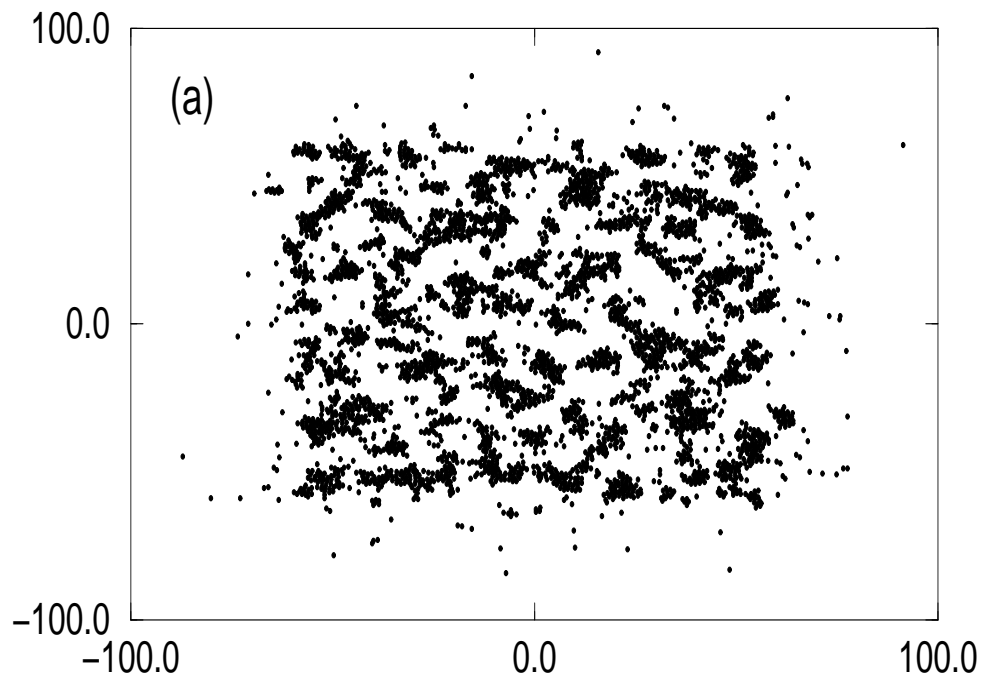


FIG. 2. The configuration of the particles at (a) 1000 and (b) 5000 time steps for the same parameters in Fig. 1 and $R = 0.43$.

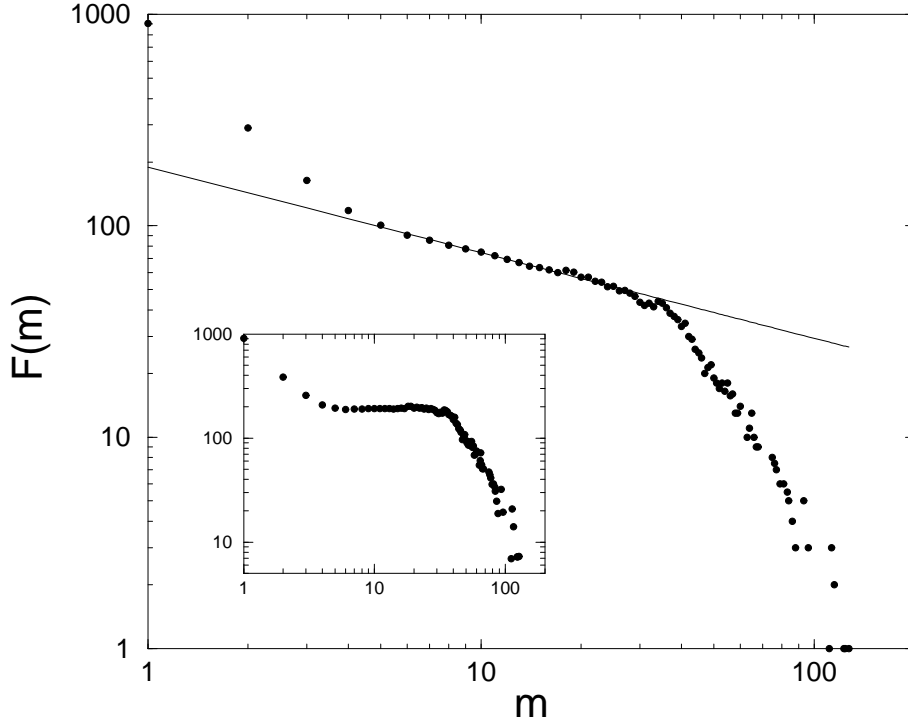


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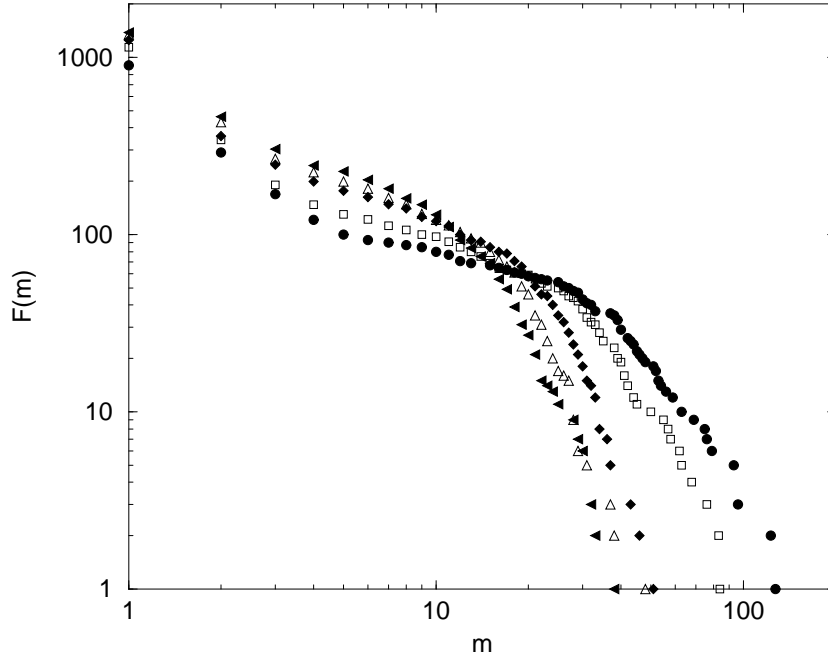


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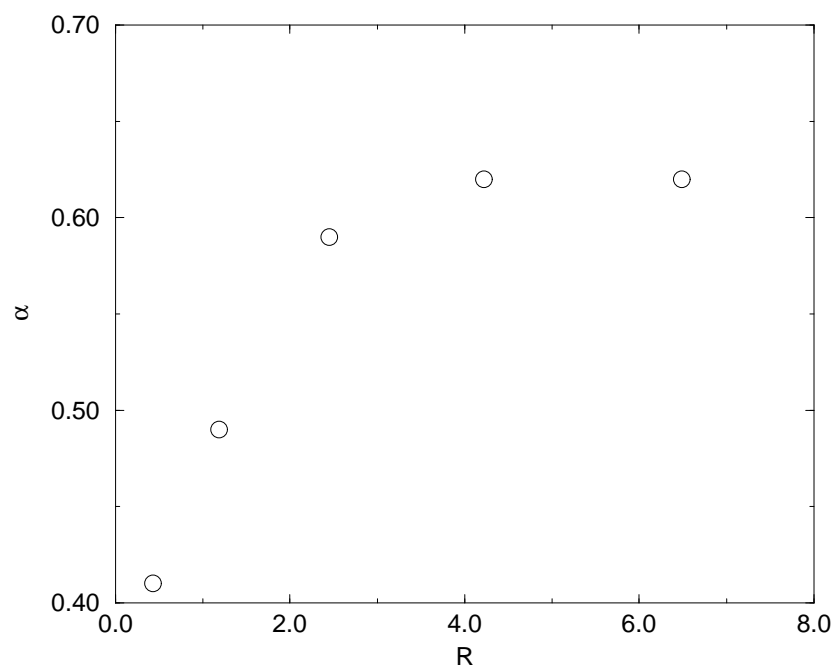


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